Ideal Gas Thermodynamic Functions of the Isotopic Hydrogen Cyanides[1]

Joe C. Bradley, Lester Haar,[2] and Abraham S. Friedman

The ideal gas thermodynamic functions for HCN, DCN, and TCN were calculated from molecular data. The recent spectroscopic data for HCN and DCN by Allen [1][3] and Douglas and Sharma [2] were employed. The zero frequencies of TCN were obtained by a normal coordinate treatment. The partition functions are obtained in closed form. The calculations include high-temperature corrections for vibrational anharmonicity, rotation-vibration coupling, centrifugal stretching, and azimuthal quantum effects, and low-temperature corrections for nonclassical rotation. The statistical calculations were performed on the Standards Electronic Automatic Computer (SEAC). Tables of C_p°/R, $(H^\circ-E_0^\circ)/RT$, $-(F^\circ-E_0^\circ)/RT$, and S°/R have been calculated at small temperature intervals from 50° to 5,000° K.

1. Introduction

The procedure developed in earlier papers [3,4,5] for high-speed machine computation of the thermodynamic functions of molecules in the ideal gas state was used. The partition function is written in a factored form to include corrections for vibrational anharmonicity, rotation-vibration coupling, centrifugal stretching, nonclassical rotation, and azimuthal quantum effects. The expression for the factored internal partition function is

$$Q=\frac{1}{S}\left[\prod_i(1-e^{-u_i})^{d_i}\right]\left[\frac{kT}{hcB_e}\right]\left[1+\rho T\right]\left[\prod_i\left(1+\frac{d_i\delta_i}{e^{u_i}-1}\right)\right]\left[\prod_{i\leq j}(1+f_{ij})\right]\left[1+\frac{\theta_1}{T}+\frac{\theta_2}{T^2}\right]$$

where

$$\rho=(2kD)/hcB_e^2,$$

$$\theta_1=\frac{1}{3}(hcB_e)/k, \theta_2=\frac{1}{15}(hcB_e/k)^2$$

and

$$f_{ij}=\frac{d_i(d_j+\delta_{ij})X'_{ij}(hc/kT)}{(e^{u_i}-1)(e^{u_i}-1)}, X'_{ij}=X_{ij}+g_{ij}/3.$$

In these expressions the δ_i represent rotation-vibration coupling constants, the X_{ij} are the anharmonic constants, g_{22} is an anharmonic constant for the doubly degenerate vibration, ω_2, and δ_{ij} is the kronecker delta. Pennington and Kobe's method [6] of including the g_{22} term in the partition function was used. The other symbols and constants have their usual meaning (see e. g., [3]).

[1] This work was supported in part by the U. S. Atomic Energy Commission.
[2] Present address: Johns Hopkins University Applied Physics Laboratory.
[3] Figures in brackets indicate the literature references at the end of this paper.

2. Molecular Data

The vibrational data for HCN and DCN were recently obtained by Allen [1]. The rotational data for HCN and DCN were investigated by Douglas and Sharma [2]. The anharmonicity and rotation-vibration coupling constants were calculated for TCN using the isotope relations [3],

$$X'_{ij}=\left(\frac{\omega'_i\omega'_j}{\omega_i\omega_j}\right)X_{ij} \quad \text{and} \quad \delta'_i=\left(\frac{\omega'_i}{\omega_i}\right)\delta_i$$

where the primed quantities refer to the molecule whose X_{ij} or δ_i is to be calculated, and the unprimed quantities refer to the reference molecule. The X_{ij} and δ_i for TCN were calculated using HCN and DCN as reference molecules; the averages of these calculations were used in the tabulated results except for the constant X_{12} in which case DCN was used as a reference molecule. Approximating

$$\underset{(i\neq j)}{f_{ij}}=\frac{d_i(d_j+\delta_{ij})\frac{hc}{kT}X'_{ij}}{(e^{u_i}-1)(e^{u_j}-1)} \quad \text{by} \quad \underset{(i\neq j)}{f_{ij}}=\frac{d_i(d_j+\delta_{ij})\frac{hc}{kT}X'_{ij}}{(e^{u_k}-1)^2}$$

where $u_k^2=u_iu_j$ changes the correction factor f_{23} by 20 percent and the free energy by 1 part in 36,000 at 5,000°K. This effect is much less in the case of f_{13} and f_{12} (see [3]). The zero-order frequencies for TCN were obtained by a normal coordinate treatment.

The chemical atomic weights used in the calculations of the translational partition functions were obtained from the values listed by Wichers [7]. The isotopic mass used in the zero-point frequency and equilibrium moment of inertia calculation are listed by Mattauch and Fluegge [8]. The constants used are given in table 1.

TABLE 1. *Molecular constants*

	Units	HCN	DCN	TCN
ν_1	cm^{-1}	2100.24	1927.27	1723.90
ν_2	cm^{-1}	711.90	569.13	503.36
ν_3	cm^{-1}	3315.03	2632.33	2446.67
X_{11}	cm^{-1}	10.45	7.10	6.37
X_{22}	cm^{-1}	2.50	2.09	1.45
X_{33}	cm^{-1}	52.50	20.23	22.72
X_{12}	cm^{-1}	2.90	−2.73	−1.93
X_{13}	cm^{-1}	14.43	32.88	18.00
X_{23}	cm^{-1}	19.19	15.71	11.48
g_{22}	dimensionless	3.63	−2.00	−1.00
δ_1	dimensionless	0.00643	0.00518	0.00495
δ_2	dimensionless	−.0024	−.0035	−.0024
δ_3	dimensionless	.00727	.00854	.0066
I_e	$g\ cm^2 \times 10^{-40}$	18.846	23.093	27.029
θ_1	°K	0.7122	0.5812	0.4967
θ_2	$(°K)^2$	.2965	.1975	.1442
ρ	$(°K)^{-1} \times 10^{-6}$	1.79	1.99	1.88

3. Thermal Functions

The heat capacity, enthalpy, free energy, and entropy of HCN, DCN, and TCN are listed in tables 2, 3, and 4. The thermal functions are tabulated in dimensionless units at small intervals ranging from 50° to 5,000° K. These tables also include the first differences for the tabulated thermodynamic functions.

The uncertainty in the calculated vibrational anharmonicity and rotation-vibration coupling constants is approximately 25 percent except in the case of the anharmonic constant X_{12} for TCN in which case the sign of the constant cannot be satisfactorily predicted. The uncertainty in the vibrational and rotational fundamentals is less than 1 percent assuming negligible uncertainty in the calculated zero point vibrational frequencies. At temperatures below 1,000° K this will result in an uncertainty in the third place to the right of the decimal for the tabulated properties of these substances. The thermal functions are tabulated with more figures to permit intercomparison among the several isotopic modifications.

The contribution of the excited electronic states, significant only at the highest temperatures, have been neglected. The entropy contribution of isotopic spin and the entropy of isotopic mixing have been omitted.

Stamm, Halverson, and Whalen [9] have revised older tables of free energy for HCN which include corrections for vibrational anharmonicity, rotation-vibration coupling, centrifugal stretching, and a low-temperature correction. The results reported here are in excellent agreement with those of Stamm et al.

TABLE 2. *Ideal gas thermodynamic functions for* HCN

°K	$\frac{C_p^\circ}{R}$		$\frac{(H^\circ - E_0^\circ)}{RT}$		$\frac{-(F^\circ - E_0^\circ)}{RT}$		$\frac{S^\circ}{R}$	
50	3.50020	4	3.48581	240	14.22796	63576	17.71377	63816
60	3.50025	19	3.48821	173	14.86372	53784	18.35194	53957
70	3.50045	74	3.48994	135	15.40157	46610	18.89152	46746
80	3.50120	209	3.49129	119	15.86768	41128	19.35898	41248
90	3.50329	456	3.49249	128	16.27897	36803	19.77146	36931
100	3.50786	825	3.49378	162	16.64700	33306	20.14078	33468
110	3.51612	1301	3.49540	223	16.98007	30423	20.47547	30646
120	3.52913	1850	3.49763	309	17.28430	28007	20.78193	28317
130	3.54764	2431	3.50073	418	17.56437	25957	21.06511	26376
140	3.57195	3004	3.50491	543	17.82395	24199	21.32887	24743
150	3.60199	3539	3.51035	680	18.06595	22676	21.57630	23357
160	3.63739	4013	3.51716	823	18.29271	21346	21.80987	22169
170	3.67753	4415	3.52539	966	18.50618	20177	22.03157	21143
180	3.72168	4738	3.53505	1105	18.70795	19142	22.24301	20247
190	3.76906	4983	3.54611	1238	18.89937	18220	22.44548	19458
200	3.81890	5157	3.55849	1362	19.08157	17394	22.64007	18756
210	3.87047	5266	3.57212	1475	19.25552	16651	22.82764	18126
220	3.92313	5318	3.58687	1577	19.42203	15978	23.00891	17556
230	3.97632	5323	3.60265	1667	19.58182	15367	23.18447	17035
240	4.02955	5288	3.61933	1746	19.73549	14810	23.35482	16556
250	4.08243	5223	3.63679	1814	19.88359	14298	23.52039	16113
260	4.13467	5133	3.65494	1872	20.02658	13828	23.68153	15700
270	4.18600	5026	3.67366	1919	20.16487	13394	23.83854	15314
280	4.23627	4906	3.69286	1958	20.29882	12992	23.99169	14951
290	4.28534	4778	3.71245	1989	20.42875	12619	24.14120	14608
300	4.33313	4646	3.73235	2013	20.55494	12271	24.28729	14284
310	4.37959	4511	3.75248	2030	20.67765	11945	24.43014	13976
320	4.42471	4378	3.77279	2042	20.79711	11640	24.56990	13682
330	4.46849	4246	3.79321	2048	20.91352	11354	24.70673	13403
340	4.51096	4118	3.81370	2051	21.02706	11084	24.84076	13135
350	4.55215	3995	3.83421	2050	21.13791	10830	24.97212	12880
360	4.59210	3877	3.85471	2045	21.24621	10589	25.10092	12635
370	4.63088	3765	3.87517	2038	21.35210	10361	25.22727	12399
380	4.66853	3658	3.89555	2029	21.45572	10145	25.35127	12174
390	4.70511	3558	3.91584	2017	21.55717	9939	25.47301	11957
400	4.74069	16483	3.93602	9875	21.65656	46933	25.59259	56808
450	4.90553	14768	4.03477	9457	22.12590	43004	26.16068	52462
500	5.05321	13540	4.12935	9022	22.55594	39783	26.68530	48805
550	5.18861	12637	4.21957	8607	22.95378	37087	27.17335	45694
600	5.31499	11936	4.30565	8227	23.32465	34790	27.63030	43018
650	5.43435	11356	4.38792	7883	23.67256	32808	28.06048	40691
700	5.54792	10843	4.46675	7571	24.00064	31077	28.46740	38649
750	5.65636	10368	4.54247	7288	24.31142	29550	28.85389	36838
800	5.76004	9912	4.61535	7027	24.60692	28192	29.22228	35219
850	5.85917	9468	4.68563	6784	24.88885	26975	29.57448	33760
900	5.95386	9032	4.75347	6557	25.15860	25877	29.91208	32434
950	6.04418	8604	4.81905	6342	25.41738	24880	30.23643	31223
1000	6.13022	8184	4.88247	6138	25.66619	23971	30.54866	30109
1050	6.21207	7776	4.94386	5942	25.90590	23136	30.84976	29079
1100	6.28984	7381	5.00328	5755	26.13726	22368	31.14055	28123
1150	6.36365	7000	5.06084	5575	26.36095	21657	31.42179	27232
1200	6.43366	12921	5.11660	10637	26.57752	41379	31.69412	52016
1300	6.56287	11596	5.22297	9992	26.99131	39075	32.21428	49068
1400	6.67883	10409	5.32289	9392	27.38207	37047	32.70496	46440
1500	6.78293	9357	5.41682	8835	27.75255	35244	33.16937	44080
1600	6.87650	8431	5.50518	8318	28.10499	33627	33.61017	41945
1700	6.96081	7617	5.58836	7839	28.44126	32166	34.02963	40006
1800	7.03699	6906	5.66676	7396	28.76263	30838	34.42969	38235
1900	7.10605	6283	5.74073	6986	29.07131	29625	34.81204	36611
2000	7.16888	5737	5.81059	6606	29.36757	28511	35.17816	35118
2100	7.22626	5260	5.87666	6255	29.65268	27483	35.52934	33739
2200	7.27887	4840	5.93921	5931	29.92752	26532	35.86674	32464
2300	7.32727	4472	5.99853	5630	30.19285	25649	36.19138	31280
2400	7.37200	4147	6.05483	5352	30.44935	24826	36.50418	30179
2500	7.41347	3859	6.10836	5094	30.69761	24057	36.80598	29152
2600	7.45207	3605	6.15931	4855	30.93819	23337	37.09750	28192
2700	7.48812	3379	6.20786	4633	31.17156	22660	37.37943	27294
2800	7.52192	3177	6.25420	4426	31.39817	22024	37.65237	26451
2900	7.55370	2998	6.29846	4234	31.61841	21424	37.91688	25659
3000	7.58368	5528	6.34081	7943	31.83266	41179	38.17348	49123
3200	7.63897	5005	6.42025	7318	32.24446	39145	38.66471	46463
3400	7.68902	4577	6.49343	6771	32.63591	37309	39.12935	44080
3600	7.73479	4223	6.56114	6289	33.00901	35644	39.57015	41934
3800	7.77703	3928	6.62404	5864	33.36546	34127	39.98950	39992
4000	7.81631	3680	6.68268	5486	33.70673	32739	40.38942	38225
4200	7.85312	3469	6.73755	5150	34.03412	31463	40.77168	36613
4400	7.88781	3288	6.78905	4849	34.34876	30286	41.13781	35135
4600	7.92069	3132	6.83755	4578	34.65162	29198	41.48917	33776
4800	7.95201	2996	6.88333	4335	34.94360	28187	41.82694	32522
5000	7.98198	----	6.92669	----	35.22548	-----	42.15217	-----

TABLE 3. *Ideal gas thermodynamic functions for* DCN

°K	$\frac{C_p^\circ}{R}$		$\frac{(H^\circ-E_0^\circ)}{RT}$		$\frac{-(F^\circ-E_0^\circ)}{RT}$		$\frac{S^\circ}{R}$	
50	3.50026	43	3.48845	199	14.48342	63620	17.97188	63820
60	3.50069	187	3.49044	157	15.11963	53817	18.61008	53974
70	3.50256	528	3.49202	160	15.65781	46639	19.14983	46799
80	3.50785	1107	3.49362	213	16.12420	41160	19.61782	41373
90	3.51893	1883	3.49575	318	16.53581	36846	20.03156	37165
100	3.53776	2771	3.49894	471	16.90428	33369	20.40322	33841
110	3.56548	3673	3.50366	662	17.23797	30512	20.74163	31174
120	3.60221	4506	3.51028	875	17.54310	28130	21.05338	29005
130	3.64727	5217	3.51903	1098	17.82440	26117	21.34344	27216
140	3.69944	5779	3.53002	1319	18.08558	24398	21.61560	25717
150	3.75723	6188	3.54321	1529	18.32956	22915	21.87278	24444
160	3.81911	6453	3.55851	1721	18.55871	21624	22.11722	23345
170	3.88365	6591	3.57572	1893	18.77496	20491	22.35068	22384
180	3.94956	6624	3.59466	2042	18.97987	19489	22.57453	21531
190	4.01581	6572	3.61508	2168	19.17476	18597	22.78985	20765
200	4.08153	6455	3.63676	2272	19.36074	17798	22.99751	20070
210	4.14609	6291	3.65949	2355	19.53872	17078	23.19821	19433
220	4.20901	6094	3.68304	2420	19.70950	16425	23.39255	18845
230	4.26995	5876	3.70724	2467	19.87375	15829	23.58100	18297
240	4.32871	5646	3.73192	2500	20.03205	15285	23.76398	17785
250	4.38518	5413	3.75693	2521	20.18490	14784	23.94184	17305
260	4.43932	5183	3.78214	2530	20.33274	14321	24.11489	16852
270	4.49115	4958	3.80745	2531	20.47596	13892	24.28341	16423
280	4.54074	4743	3.83276	2523	20.61488	13493	24.44765	16017
290	4.58817	4539	3.85800	2510	20.74982	13121	24.60782	15631
300	4.63357	4348	3.88310	2491	20.88104	12773	24.76414	15264
310	4.67706	4171	3.90801	2468	21.00877	12446	24.91679	14915
320	4.71877	4006	3.93270	2443	21.13324	12139	25.06594	14582
330	4.75884	3856	3.95713	2415	21.25463	11849	25.21176	14264
340	4.79740	3718	3.98128	2385	21.37312	11575	25.35441	13960
350	4.83459	3593	4.00513	2354	21.48887	11315	25.49401	13670
360	4.87052	3479	4.02868	2322	21.60203	11069	25.63071	13392
370	4.90532	3377	4.05190	2290	21.71273	10836	25.76464	13126
380	4.93909	3284	4.07481	2258	21.82109	10613	25.89590	12872
390	4.97194	3201	4.09739	2226	21.92723	10401	26.02463	12628
400	5.00395	15029	4.11966	10673	22.03125	49146	26.15091	59820
450	5.15425	13906	4.22639	9981	22.52271	45051	26.74911	55032
500	5.29331	13197	4.32620	9396	22.97323	41678	27.29944	51074
550	5.42528	12669	4.42017	8907	23.39001	38845	27.81018	47752
600	5.55198	12195	4.50924	8493	23.77847	36431	28.28771	44924
650	5.67393	11713	4.59417	8133	24.14278	34346	28.73695	42480
700	5.79107	11204	4.67551	7813	24.48524	32525	29.16176	40339
750	5.90311	10666	4.75364	7520	24.81150	30920	29.56515	38441
800	6.00978	10110	4.82885	7246	25.12071	29493	29.94956	36740
850	6.11089	9546	4.90132	6987	25.41565	28214	30.31697	35201
900	6.20635	8986	4.97119	6739	25.69779	27059	30.66899	33799
950	6.29622	8438	5.03859	6501	25.96838	26010	31.00698	32512
1000	6.38060	7909	5.10360	6271	26.22849	25053	31.33210	31324
1050	6.45969	7405	5.16632	6049	26.47903	24174	31.64535	30223
1100	6.53375	6928	5.22681	5834	26.72077	23363	31.94758	29198
1150	6.60304	6480	5.28515	5627	26.95441	22613	32.23956	28240
1200	6.66784	11734	5.34143	10664	27.18054	43180	32.52197	53845
1300	6.78519	10288	5.44808	9926	27.61234	40742	33.06042	50668
1400	6.88807	9050	5.54734	9246	28.01976	38591	33.56711	47838
1500	6.97858	7997	5.63980	8622	28.40568	36676	34.04549	45299
1600	7.05855	7101	5.72602	8051	28.77245	34958	34.49848	43009
1700	7.12957	6340	5.80654	7529	29.12203	33404	34.92858	40934
1800	7.19298	5692	5.88183	7053	29.45608	31992	35.33792	39045
1900	7.24990	5138	5.95236	6618	29.77601	30701	35.72838	37320
2000	7.30129	4664	6.01855	6221	30.08303	29516	36.10158	35737
2100	7.34793	4256	6.08076	5858	30.37819	28424	36.45896	34282
2200	7.39049	3903	6.13934	5525	30.66244	27413	36.80178	32939
2300	7.42953	3598	6.19460	5221	30.93657	26475	37.13117	31696
2400	7.46551	3332	6.24681	4942	31.20132	25601	37.44814	30544
2500	7.49884	3100	6.29624	4685	31.45734	24786	37.75358	29472
2600	7.52985	2896	6.34309	4449	31.70521	24023	38.04830	28472
2700	7.55882	2717	6.38759	4231	31.94544	23307	38.33303	27539
2800	7.58599	2558	6.42991	4031	32.17851	22634	38.60843	26665
2900	7.61158	2418	6.47022	3845	32.40486	22000	38.87508	25845
3000	7.63576	4473	6.50867	7186	32.62486	42238	39.13354	49425
3200	7.68049	4070	6.58053	6591	33.04725	40094	39.62779	46686
3400	7.72119	3742	6.64645	6076	33.44820	38164	40.09466	44240
3600	7.75862	3473	6.70721	5626	33.82984	36416	40.53706	42042
3800	7.79335	3249	6.76348	5231	34.19401	34826	40.95749	40058
4000	7.82584	3060	6.81579	4883	34.54228	33373	41.35807	38257
4200	7.85645	2900	6.86462	4574	34.87602	32041	41.74064	36615
4400	7.88545	2762	6.91037	4300	35.19643	30813	42.10680	35113
4600	7.91308	2643	6.95337	4054	35.50456	29679	42.45794	33734
4800	7.93951	2538	6.99391	3833	35.80136	28629	42.79528	32462
5000	7.96490	------	7.03225	------	36.08765	-------	43.11990	-------

TABLE 4. *Ideal gas thermodynamic functions for* TCN

°K	$\frac{C_p^\circ}{R}$		$\frac{(H^\circ-E_0^\circ)}{RT}$		$\frac{(-F^\circ-E_0^\circ)}{RT}$		$\frac{S^\circ}{R}$	
50	3.50031	89	3.49015	174	14.69139	63649	18.18154	63824
60	3.50120	345	3.49189	153	15.32789	53839	18.81979	53992
70	3.50466	878	3.49343	188	15.86628	46659	19.35971	46848
80	3.51344	1686	3.49531	286	16.33288	41184	19.82819	41470
90	3.53031	2676	3.49818	446	16.74472	36878	20.24290	37325
100	3.55708	3720	3.50264	656	17.11351	33412	20.61615	34068
110	3.59428	4700	3.50920	898	17.44763	30570	20.95684	31469
120	3.64129	5538	3.51819	1155	17.75334	28204	21.27153	29359
130	3.69667	6195	3.52974	1410	18.03539	26208	21.56513	27618
140	3.75862	6662	3.54384	1651	18.29747	24505	21.84132	26156
150	3.82525	6954	3.56036	1871	18.54252	23036	22.10288	24908
160	3.89479	7093	3.57908	2035	18.77289	21759	22.35197	23824
170	3.96572	7107	3.59973	2230	18.99048	20637	22.59022	22868
180	4.03680	7024	3.62204	2368	19.19686	19646	22.81890	22014
190	4.10704	6870	3.64572	2479	19.39332	18762	23.03905	21241
200	4.17574	6665	3.67051	2565	19.58095	17970	23.25147	20535
210	4.24240	6429	3.69617	2629	19.76065	17255	23.45683	19885
220	4.30670	6174	3.72247	2675	19.93320	16605	23.65568	19281
230	4.36844	5913	3.74922	2704	20.09926	16013	23.84849	18717
240	4.42758	5653	3.77626	2719	20.25940	15470	24.03567	18189
250	4.48411	5399	3.80346	2722	20.41411	14970	24.21757	17693
260	4.53811	5158	3.83068	2716	20.56381	14508	24.39450	17224
270	4.58969	4929	3.85785	2702	20.70889	14079	24.56674	16781
280	4.63899	4717	3.88487	2682	20.84968	13679	24.73456	16361
290	4.68617	4520	3.91169	2657	20.98648	13306	24.89817	15963
300	4.73138	4340	3.93827	2628	21.11954	12956	25.05781	15585
310	4.77478	4176	3.96456	2597	21.24910	12628	25.21366	15225
320	4.81655	4027	3.99053	2564	21.37538	12318	25.36592	14883
330	4.85682	3892	4.01618	2530	21.49857	12027	25.51475	14557
340	4.89574	3771	4.04148	2494	21.61884	11751	25.66033	14246
350	4.93346	3662	4.06643	2459	21.73636	11490	25.80279	13949
360	4.97008	3564	4.09102	2424	21.85126	11242	25.94229	13666
370	5.00572	3476	4.11526	2389	21.96368	11006	26.07895	13395
380	5.04049	3397	4.13916	2354	22.07375	10782	26.21291	13137
390	5.07447	3327	4.16270	2321	22.18157	10568	26.34428	12889
400	5.10774	15795	4.18592	11131	22.28725	49953	26.47317	61084
450	5.26569	14778	4.29723	10430	22.78678	45821	27.08402	56251
500	5.41348	14037	4.40154	9842	23.24500	42417	27.64654	52259
550	5.55385	13388	4.49996	9344	23.66917	39558	28.16914	48903
600	5.68774	12749	4.59341	8912	24.06476	37121	28.65817	46034
650	5.81523	12091	4.68253	8526	24.43597	35015	29.11851	43542
700	5.93615	11414	4.76780	8173	24.78613	33175	29.55393	41348
750	6.05030	10728	4.84953	7843	25.11788	31550	29.96742	39393
800	6.15758	10046	4.92797	7531	25.43339	30103	30.36136	37635
850	6.25805	9380	5.00329	7234	25.73442	28804	30.73771	36038
900	6.35186	8740	5.07563	6949	26.02246	27630	31.09810	34579
950	6.43926	8132	5.14513	6676	26.29876	26562	31.44389	33238
1000	6.52059	7560	5.21189	6414	26.56438	25585	31.77628	31999
1050	6.59620	7026	5.27603	6162	26.82023	24687	32.09627	30849
1100	6.66647	6531	5.33766	5921	27.06711	23858	32.40477	29779
1150	6.73178	6074	5.39687	5690	27.30569	23089	32.70256	28780
1200	6.79253	10920	5.45377	10728	27.53659	44082	32.99037	54810
1300	6.90173	9500	5.56105	9923	27.97742	41579	33.53847	51503
1400	6.99673	8309	5.66028	9192	28.39322	39369	34.05350	48562
1500	7.07982	7312	5.75221	8530	28.78691	37399	34.53913	45930
1600	7.15295	6476	5.83752	7932	29.16091	35630	34.99843	43562
1700	7.21772	5774	5.91684	7390	29.51721	34031	35.43406	41421
1800	7.27546	5181	5.99075	6900	29.85753	32577	35.84828	39477
1900	7.32728	4679	6.05975	6456	30.18330	31248	36.24306	37705
2000	7.37407	4251	6.12431	6054	30.49579	30028	36.62011	36082
2100	7.41659	3886	6.18485	5688	30.79607	28904	36.98093	34593
2200	7.45545	3572	6.24174	5355	31.08512	27865	37.32686	33220
2300	7.49118	3301	6.29530	5052	31.36377	26900	37.65907	31952
2400	7.52419	3066	6.34582	4775	31.63277	26002	37.97860	30778
2500	7.55485	2861	6.39358	4522	31.89280	25164	38.28638	29687
2600	7.58347	2682	6.43880	4289	32.14445	24381	38.58325	28671
2700	7.61030	2525	6.48169	4076	32.38826	23646	38.86996	27722
2800	7.63555	2386	6.52246	3879	32.62473	22956	39.14719	26836
2900	7.65941	2263	6.56125	3698	32.85430	22306	39.41556	26005
3000	7.68205	4209	6.59824	6907	33.07736	42807	39.67561	49715
3200	7.72414	3858	6.66731	6331	33.50544	40613	40.17276	46944
3400	7.76273	3572	6.73063	5834	33.91157	38638	40.64221	44472
3600	7.79845	3338	6.78897	5401	34.29796	36852	41.08694	42254
3800	7.83183	3142	6.84299	5023	34.66648	35229	41.50948	40252
4000	7.86326	2978	6.89323	4690	35.01878	33746	41.91201	38437
4200	7.89304	2837	6.94013	4396	35.35625	32388	42.29639	36784
4400	7.92142	2717	6.98410	4134	35.68013	31137	42.66423	35272
4600	7.94859	2612	7.02545	3901	35.99151	29983	43.01696	33884
4800	7.97471	2520	7.06446	3691	36.29134	28914	43.35580	32605
5000	7.99991	------	7.10138	------	36.58048	-------	43.68186	-------

378088—56——3

4. References

[1] H. C. Allen (private communication).
[2] A. E. Douglas and D. Sharma, J. Chem. Phys. **21,** 448 (1953).
[3] A. S. Friedman and L. Haar, J. Chem. Phys. **22,** 2051 (1954).
[4] L. Harr and A. S. Friedman, J. Chem. Phys. **23,** 869 (1955).
[5] L. Haar, J. C. Bradley, and A. S. Friedman, J. Research NBS **55,** 285 (1955) RP2631.
[6] R. E. Pennington and K. A. Kobe, J. Chem. Phys. **22,** 1442 (1954).
[7] E. Wichers, J. Am. Chem. Soc. **74,** 2447 (1952).
[8] J. Mattauch and S. Fluegge, Nuclear physics tables and an introduction to nuclear physics (Interscience Publishers, Inc., New York, N. Y., 1946).
[9] Stamm, Halverson, and Whalen, J. Chem. Phys. **17,** 104 (1949).

WASHINGTON, December 12, 1955.